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COMPUTED HEATS OF FORMATION

by

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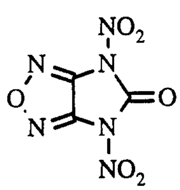
13. ABSTRACT (Maximum 200 words)

Computed heats of formation for **1 - 8.**



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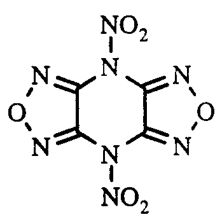

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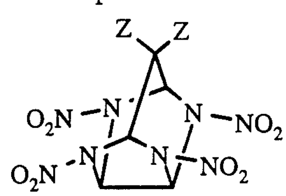
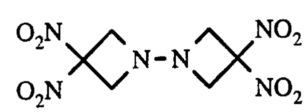


3: Z = H
4: Z = NO_2
5: Z = NF_2



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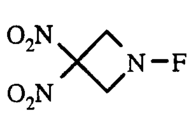

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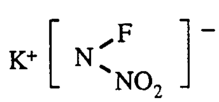

8

1: ΔH_f^{298K}(solid) = 231 cal/g
2: ΔH_f^{298K}(solid) = 491 cal/g
3: ΔH_f^{298K}(solid) = 150 cal/g
4: ΔH_f^{298K}(solid) = 157 cal/g
5: ΔH_f^{298K}(solid) = 132 cal/g
6: ΔH_f^{298K}(solid) = 235 cal/g
7: ΔH_f^{298K}(solid) = 1.5 cal/g
8: ΔH_f^{298K}(solid) = –584 cal/g

14. SUBJECT TERMS
Energetic compounds; heats of formation

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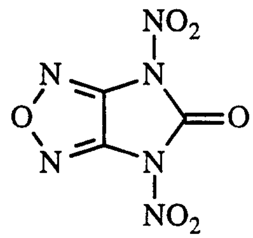
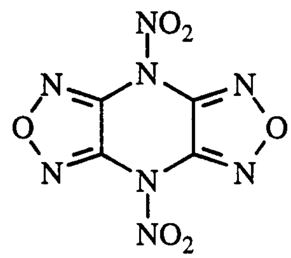
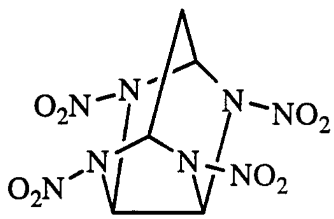
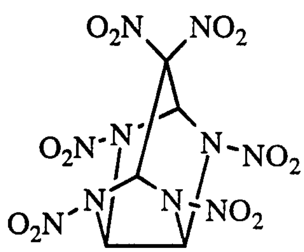
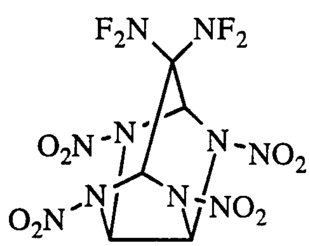
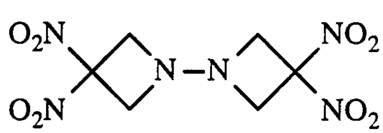
Unclassified	Unclassified	Unclassified	Unlimited

We have computed heats of formation for compounds **1** - **8** (Table 1). The first five are target compounds proposed by M. Trudell (University of New Orleans); **6** - **8** have recently been prepared by R. Schmitt and J. Bottaro (SRI). For the molecular systems **1** - **7**, we used our density functional procedure to obtain gas phase heats of formation, which were converted to liquid and solid state values by subtracting, respectively, the heats of vaporization and sublimation. The latter are determined by means of relationships that we have developed involving the computed electrostatic potential on the molecular surface [2,3]. (Vibrational energies were obtained from the molecular stoichiometries [4].) For the ionic solid **8**, the heat of formation was calculated using the lattice enthalpy and the gas phase heats of formation of the positive and negative ions; the lattice enthalpy was computed from our recently-developed relationship involving anionic surface electrostatic potentials [5]. For comparison, the experimental solid phase heats of formation of HMX and RDX are, respectively, 60.4 cal/g and 76.1 cal/g [6].

References:

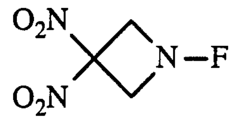
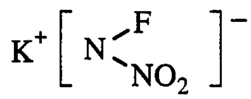
1. D. Habibollahzadeh, M. E. Grice, M. C. Concha, J. S. Murray and P. Politzer, J. Comp. Chem. **16**, 654 (1995).
2. J. S. Murray and P. Politzer, *Quantitative Treatments of Solute/Solvent Interactions*, J.S . Murray and P. Politzer, Eds., Elsevier, Amsterdam, 1994, ch. 8.
3. P. Politzer, J. S. Murray, M. E. Grice, M. DeSalvo and E. Miller, Mol. Phys. **91**, 923 (1997).
4. M. E. Grice and P. Politzer, Chem. Phys. Lett. **244**, 295 (1995).
5. P. Politzer and J. S. Murray, J. Phys. Chem. A, **102**, 1018 (1998).
6. J. Köhler and R. Meyer, Explosives, 4th ed., VCH Publishers, New York, 1993.

Table 1. Computed heats of formation.

1		ΔH_f^{298K} (gas) = 73.6 kcal/mole = 341 cal/g ΔH_f^{298K} (liquid) = 60.0 kcal/mole = 278 cal/g ΔH_f^{298K} (solid) = 49.8 kcal/mole = 231 cal/g
2		ΔH_f^{298K} (gas) = 155 kcal/mole = 604 cal/g ΔH_f^{298K} (liquid) = 139 kcal/mole = 544 cal/g ΔH_f^{298K} (solid) = 126 kcal/mole = 491 cal/g
3		ΔH_f^{298K} (gas) = 80.6 kcal/mole = 263 cal/g ΔH_f^{298K} (liquid) = 64.3 kcal/mole = 210 cal/g ΔH_f^{298K} (solid) = 45.8 kcal/mole = 150 cal/g
4		ΔH_f^{298K} (gas) = 104 kcal/mole = 264 cal/g ΔH_f^{298K} (liquid) = 87.5 kcal/mole = 221 cal/g ΔH_f^{298K} (solid) = 62.2 kcal/mole = 157 cal/g
5		ΔH_f^{298K} (gas) = 96.5 kcal/mole = 236 cal/g ΔH_f^{298K} (liquid) = 79.1 kcal/mole = 194 cal/g ΔH_f^{298K} (solid) = 54.0 kcal/mole = 132 cal/g
6		ΔH_f^{298K} (gas) = 108 kcal/mole = 370 cal/g ΔH_f^{298K} (liquid) = 91.1 kcal/mole = 312 cal/g ΔH_f^{298K} (solid) = 68.7 kcal/mole = 235 cal/g

(continued)

Table 1. Computed heats of formation (continued).

7		ΔH_f^{298K} (gas) = 20.5 kcal/mole = 124 cal/g ΔH_f^{298K} (liquid) = 8.23 kcal/mole = 49.8 cal/g ΔH_f^{298K} (solid) = 0.24 kcal/mole = 1.5 cal/g
8		ΔH_f^{298K} (solid) = –69.0 kcal/mole = –584 cal/g